



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:03 PM BST

PDB ID : 4I50
Title : Crystal structure of tubulin-stathmin-TTL-Epothilone A complex
Authors : Prota, A.E.; Bargsten, K.; Zurwerra, D.; Field, J.J.; Diaz, J.F.; Altmann, K.H.; Steinmetz, M.O.
Deposited on : 2012-11-28
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

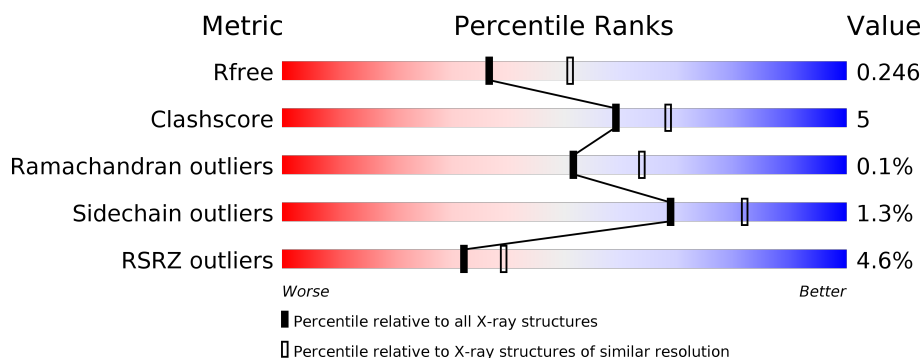
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>89%</div> <div>8%</div> <div>•</div> </div>
1	C	451	<div> <div>3%</div> <div>87%</div> <div>10%</div> <div>•</div> </div>
2	B	445	<div> <div>4%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
2	D	445	<div> <div>2%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
3	E	143	<div> <div>3%</div> <div>77%</div> <div>9%</div> <div>14%</div> </div>
4	F	384	<div> <div>17%</div> <div>67%</div> <div>11%</div> <div>•</div> <div>21%</div> </div>

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 34573 atoms, of which 16917 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	436	Total	C	H	N	O	S	0	0	0
			6740	2155	3333	580	650	22			
1	C	440	Total	C	H	N	O	S	0	10	0
			6890	2201	3412	586	666	25			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	422	Total	C	H	N	O	S	0	2	0
			6555	2092	3225	569	643	26			
2	D	430	Total	C	H	N	O	S	0	4	0
			6690	2132	3292	582	657	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	0	0
			2047	625	1033	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	CLONING ARTIFACT	UNP P63043
E	4	ALA	SER	CLONING ARTIFACT	UNP P63043

- Molecule 4 is a protein called Tubulin Tyrosine Ligase, TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	303	Total	C	H	N	O	S	0	0	0
			4964	1597	2481	423	450	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	EXPRESSION TAG	UNP E1BQ43
F	380	HIS	-	EXPRESSION TAG	UNP E1BQ43
F	381	HIS	-	EXPRESSION TAG	UNP E1BQ43
F	382	HIS	-	EXPRESSION TAG	UNP E1BQ43
F	383	HIS	-	EXPRESSION TAG	UNP E1BQ43
F	384	HIS	-	EXPRESSION TAG	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	2	Total	Mg	0	0
			2	2		

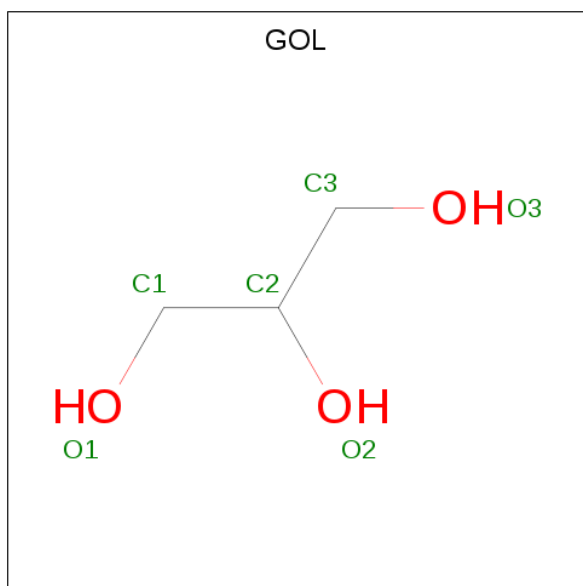
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Ca	0	0
			1	1		
7	A	2	Total	Ca	0	0
			2	2		
7	C	3	Total	Ca	0	0
			3	3		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



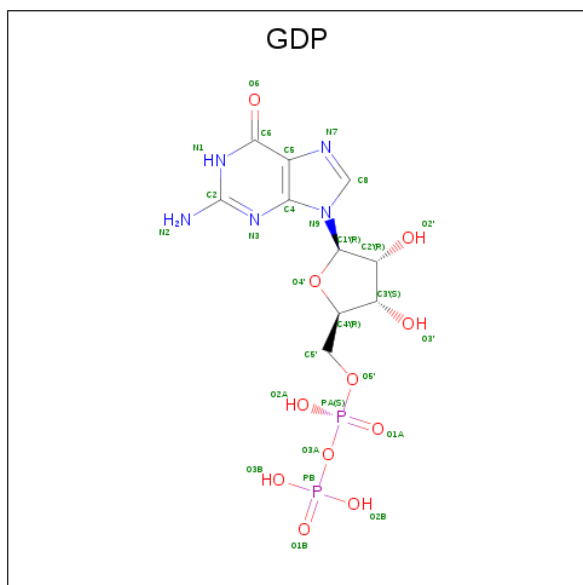
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	H	O	0	0
			14	3	8	3		
9	A	1	Total	C	H	O	0	0
			14	3	8	3		

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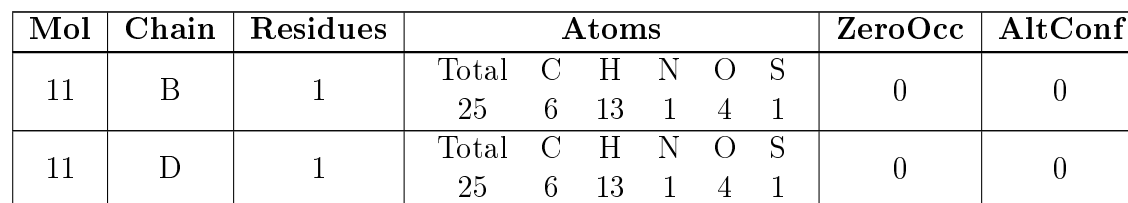
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		
10	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

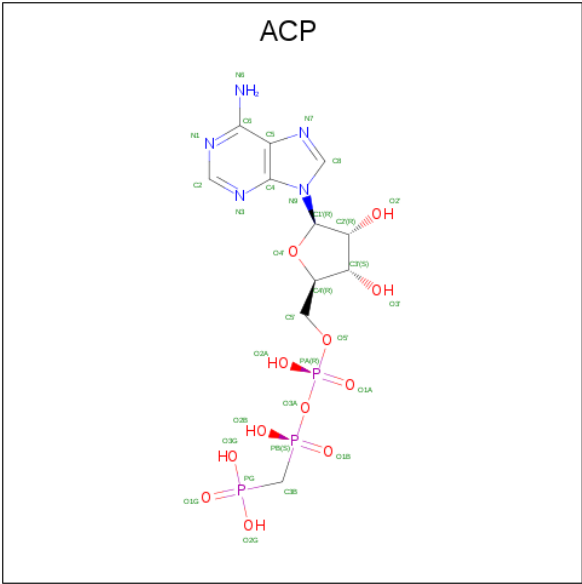


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- Chemical structure of EP (Ergosterol) is shown, highlighting stereochemistry. The structure includes a steroid nucleus with a double bond at C5-C6, a methyl group at C10, and a side chain at C13. Stereochemistry is indicated by wedged and dashed bonds. Key atoms are labeled: C1-C16, O1-O8, S1, N20, H27, H24, and C27(R). The structure is a complex polycyclic molecule with a side chain containing a double bond and a methyl group.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	D	1	Total	C	H	N	O	S	0	0
			73	26	39	1	6	1		

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- WORLD WIDE
PDB
PROTEIN DATA BANK

letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	F	1	Total	C	H	N	O	P	
			43	11	12	5	12	3	

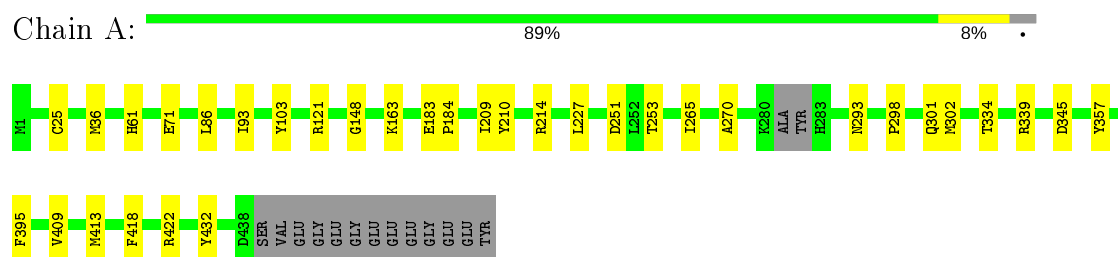
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	63	Total	O	0	0
			63	63		
14	B	50	Total	O	0	0
			50	50		
14	C	117	Total	O	0	0
			117	117		
14	D	40	Total	O	0	0
			40	40		
14	E	16	Total	O	0	0
			16	16		
14	F	20	Total	O	0	0
			20	20		

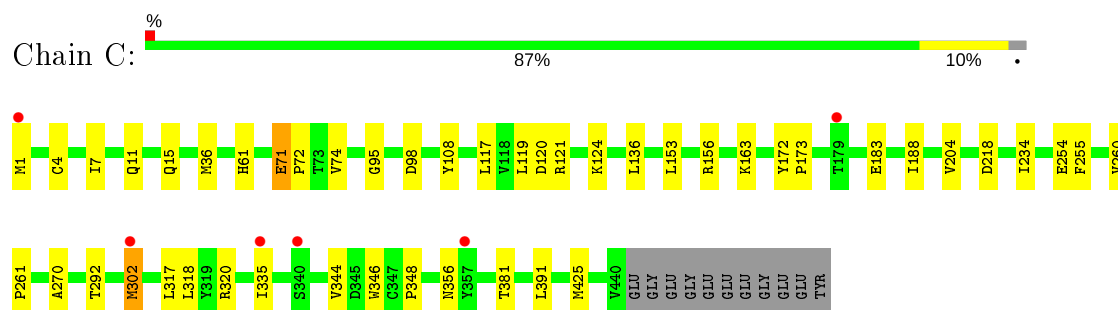
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

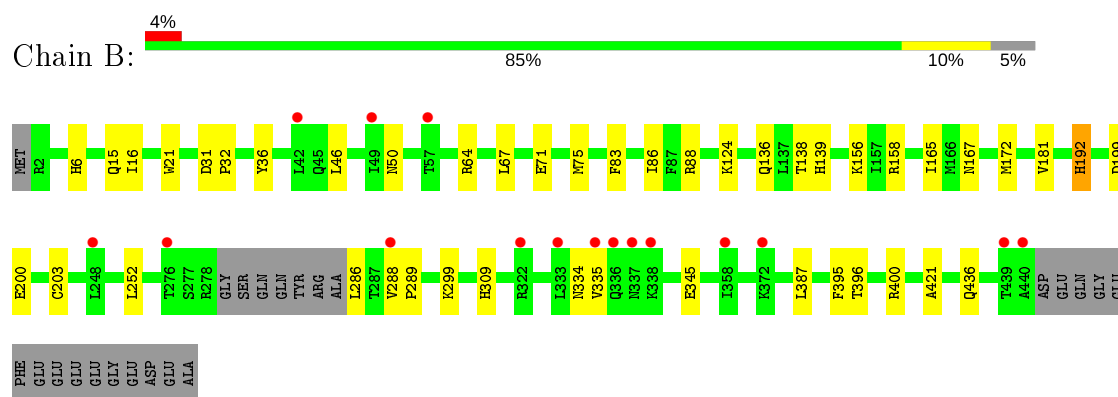
- Molecule 1: Tubulin alpha-1B chain



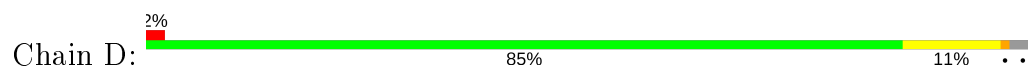
- Molecule 1: Tubulin alpha-1B chain

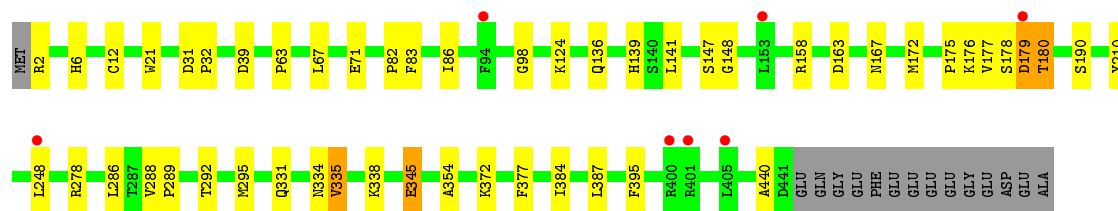


- Molecule 2: Tubulin beta-2B chain

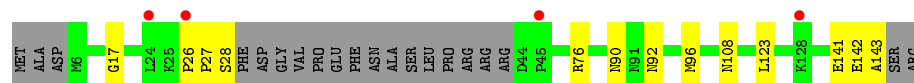
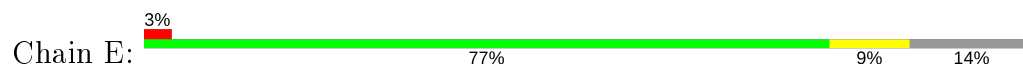


- Molecule 2: Tubulin beta-2B chain

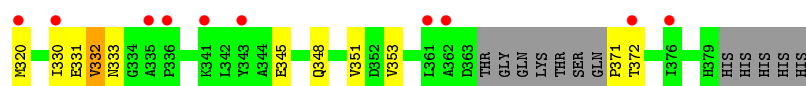
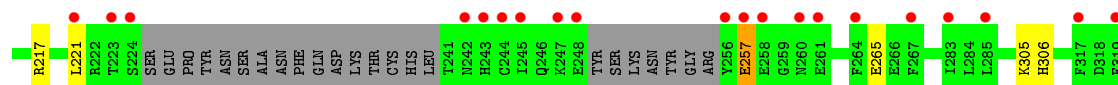
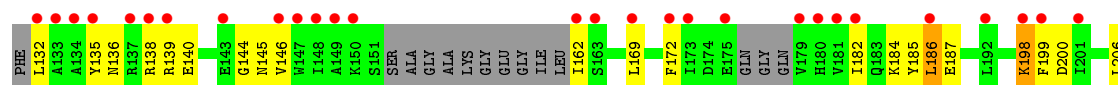
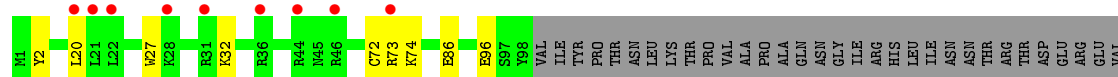




● Molecule 3: Stathmin-4



● Molecule 4: Tubulin Tyrosine Ligase, TTL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.62Å 155.13Å 180.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.56 – 2.30 77.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.56-2.30) 100.0 (77.98-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.191 , 0.246 0.191 , 0.246	Depositor DCC
R_{free} test set	6505 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	34573	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, CL, CA, GTP, ACP, MES, EP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.32	0/3483	0.49	0/4726
1	C	0.36	0/3588	0.50	0/4871
2	B	0.32	0/3409	0.47	0/4617
2	D	0.30	0/3485	0.46	0/4720
3	E	0.30	0/1022	0.40	0/1356
4	F	0.28	0/2535	0.45	0/3418
All	All	0.32	0/17522	0.47	0/23708

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3407	3333	3320	19	0
1	C	3478	3412	3387	31	0
2	B	3330	3225	3215	33	0
2	D	3398	3292	3282	34	0
3	E	1014	1033	1029	10	0
4	F	2483	2481	2472	37	0
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	2	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	3	0	0	0	0
8	A	1	0	0	1	0
9	A	12	16	16	0	0
9	D	6	8	8	0	0
10	B	28	10	12	1	0
10	D	28	10	12	1	0
11	B	12	13	13	2	0
11	D	12	13	13	2	0
12	D	34	39	38	1	0
13	F	31	12	14	2	0
14	A	63	0	0	0	0
14	B	50	0	0	5	0
14	C	117	0	0	2	0
14	D	40	0	0	0	0
14	E	16	0	0	1	0
14	F	20	0	0	0	0
All	All	17656	16917	16855	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (159) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.25	0.77
1:C:254:GLU:OE1	14:C:717:HOH:O	2.08	0.71
2:D:331:GLN:O	2:D:335:VAL:HG23	1.91	0.70
4:F:331:GLU:OE1	4:F:333:ASN:ND2	2.27	0.67
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.80	0.64
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.37	0.63
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.39	0.62
1:C:72:PRO:HD3	1:C:95:GLY:O	2.01	0.61
2:B:15:GLN:NE2	10:B:501:GDP:O6	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:CZ	11:B:504:MES:H21	2.30	0.61
12:D:504:EP:H62	12:D:504:EP:H13	1.82	0.60
2:D:136:GLN:HA	2:D:167:ASN:O	2.02	0.59
2:B:199:ASP:OD1	11:B:504:MES:H52	2.02	0.58
2:B:50:ASN:O	2:B:64:ARG:NH2	2.34	0.58
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.38	0.58
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.34	0.57
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.57
2:D:82:PRO:O	2:D:83:PHE:HB2	2.06	0.56
4:F:96:GLU:OE2	4:F:184:LYS:NZ	2.39	0.56
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.41	0.55
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.88	0.55
4:F:138:ARG:HD3	4:F:145:ASN:HA	1.87	0.55
2:B:181:VAL:HG23	1:C:348:PRO:CG	2.37	0.54
4:F:206:LEU:HD23	4:F:353:VAL:CG2	2.38	0.54
4:F:371:PRO:HA	4:F:372:THR:HB	1.90	0.54
1:A:293:ASN:OD1	1:A:339:ARG:NH1	2.42	0.53
2:B:387:LEU:C	2:B:387:LEU:HD23	2.28	0.53
2:D:163:ASP:HA	11:D:503:MES:C7	2.38	0.53
2:D:331:GLN:O	2:D:335:VAL:CG2	2.57	0.53
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.44	0.53
4:F:371:PRO:CA	4:F:372:THR:HB	2.39	0.53
4:F:162:ILE:HD12	4:F:162:ILE:N	2.23	0.52
4:F:217:ARG:NH2	4:F:345:GLU:OE2	2.43	0.52
4:F:200:ASP:OD1	13:F:401:ACP:O3'	2.28	0.52
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.91	0.52
2:D:141:LEU:HD12	2:D:172:MET:SD	2.50	0.51
2:D:292:THR:CG2	2:D:335:VAL:HG21	2.41	0.51
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.91	0.51
2:D:158:ARG:HG2	3:E:123:LEU:HD11	1.92	0.51
2:B:309:HIS:O	2:B:436:GLN:NE2	2.45	0.50
2:D:334:ASN:O	2:D:338:LYS:HG2	2.12	0.50
2:D:163:ASP:HA	11:D:503:MES:H71	1.93	0.50
1:C:1:MET:HE3	14:C:696:HOH:O	2.11	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CE2	2.47	0.49
3:E:108:ASN:ND2	14:E:206:HOH:O	2.45	0.49
2:D:286:LEU:HD23	2:D:372:LYS:CG	2.41	0.49
2:D:83:PHE:O	2:D:86:ILE:HG22	2.13	0.49
3:E:141:GLU:O	3:E:143:ALA:N	2.43	0.49
4:F:198:LYS:CG	4:F:199:PHE:N	2.75	0.49
2:B:136:GLN:HA	2:B:167:ASN:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:257:GLU:O	4:F:257:GLU:CG	2.60	0.49
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.95	0.49
1:A:270:ALA:HB3	1:A:302:MET:HG2	1.95	0.48
2:B:286:LEU:O	2:B:286:LEU:HG	2.13	0.48
2:D:124:LYS:C	2:D:124:LYS:HD3	2.34	0.48
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.95	0.48
2:D:387:LEU:C	2:D:387:LEU:HD23	2.33	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.48
2:D:286:LEU:HD23	2:D:372:LYS:HG2	1.95	0.48
4:F:146:VAL:CG1	4:F:162:ILE:CG2	2.92	0.48
1:A:345:ASP:N	1:A:345:ASP:OD1	2.46	0.48
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.44	0.48
4:F:138:ARG:CZ	4:F:184:LYS:HE3	2.43	0.48
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.49	0.47
2:D:177:VAL:HG12	2:D:177:VAL:O	2.14	0.47
4:F:144:GLY:HA3	4:F:145:ASN:HB2	1.96	0.47
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.95	0.47
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.50	0.47
2:B:192:HIS:CD2	2:B:421:ALA:HA	2.49	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.47
2:B:67:LEU:N	2:B:67:LEU:HD12	2.30	0.47
4:F:132:LEU:O	4:F:135:TYR:N	2.47	0.47
2:B:124:LYS:HD3	2:B:124:LYS:C	2.35	0.47
4:F:182:ILE:HG23	4:F:182:ILE:O	2.15	0.46
1:C:173:PRO:HB3	1:C:183:GLU:OE2	2.16	0.46
2:B:396:THR:O	2:B:400:ARG:HG3	2.15	0.46
2:D:147[A]:SER:OG	2:D:148:GLY:N	2.48	0.46
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.46	0.46
1:A:25:CYS:SG	1:A:86:LEU:HD21	2.56	0.46
2:B:334:ASN:CB	14:B:623:HOH:O	2.64	0.46
1:C:317:LEU:C	1:C:318:LEU:HD23	2.36	0.46
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.46
4:F:2:TYR:HB3	4:F:27:TRP:CZ3	2.51	0.46
1:A:183:GLU:N	1:A:184:PRO:CD	2.79	0.45
2:B:156:LYS:HD3	3:E:76:ARG:CZ	2.45	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.16	0.45
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.51	0.45
1:C:11:GLN:O	1:C:15:GLN:HG3	2.17	0.45
1:C:270:ALA:CB	1:C:302[B]:MET:SD	3.05	0.45
1:C:318:LEU:N	1:C:318:LEU:HD23	2.32	0.45
2:B:334:ASN:HB3	14:B:623:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.52	0.45
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.98	0.45
1:C:163:LYS:HG2	3:E:90:ASN:OD1	2.17	0.45
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.99	0.44
2:B:71:GLU:HG2	14:B:612:HOH:O	2.16	0.44
2:D:292:THR:CG2	2:D:335:VAL:CG2	2.95	0.44
4:F:136:ASN:O	4:F:140:GLU:N	2.51	0.44
4:F:72:CYS:SG	4:F:332:VAL:HG23	2.57	0.44
4:F:185:TYR:O	4:F:186:LEU:C	2.56	0.44
1:A:357:TYR:CE1	3:E:17:GLY:HA2	2.53	0.44
2:D:175:PRO:HA	2:D:178:SER:HB3	1.98	0.44
4:F:138:ARG:HG2	4:F:144:GLY:HA3	2.00	0.43
4:F:257:GLU:HG3	4:F:257:GLU:O	2.18	0.43
2:B:288:VAL:N	2:B:289:PRO:CD	2.81	0.43
2:B:83:PHE:O	2:B:86:ILE:HG22	2.18	0.43
1:A:298:PRO:HA	1:A:301:GLN:CD	2.38	0.43
2:B:299:LYS:HD2	2:B:299:LYS:N	2.34	0.43
4:F:138:ARG:NH2	4:F:184:LYS:CE	2.82	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.43
2:B:75:MET:N	14:B:642:HOH:O	2.47	0.43
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.99	0.43
4:F:206:LEU:HD23	4:F:353:VAL:HG21	2.01	0.43
2:D:176:LYS:HD3	2:D:210:TYR:CD1	2.54	0.43
1:C:204:VAL:HG22	1:C:302[B]:MET:HE3	2.01	0.42
1:A:409:VAL:HA	1:A:413:MET:O	2.19	0.42
2:B:395:PHE:CD2	2:B:395:PHE:C	2.92	0.42
1:A:395:PHE:CD2	1:A:422:ARG:HD3	2.54	0.42
1:C:117:LEU:HD11	1:C:121:ARG:NH1	2.34	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.42
2:D:179:ASP:C	2:D:180:THR:CG2	2.88	0.42
2:B:167:ASN:OD1	2:B:200:GLU:HG3	2.19	0.42
2:B:36:TYR:CD2	2:B:46:LEU:HD11	2.54	0.42
4:F:185:TYR:O	4:F:187:GLU:N	2.52	0.42
4:F:198:LYS:HG3	4:F:199:PHE:N	2.35	0.42
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.50	0.42
4:F:138:ARG:NH2	4:F:184:LYS:HE2	2.34	0.42
4:F:139:ARG:HD2	4:F:139:ARG:HA	1.93	0.42
4:F:20:LEU:CD2	4:F:348:GLN:OE1	2.68	0.42
3:E:26:PRO:O	3:E:28:SER:N	2.52	0.41
1:A:163:LYS:HB2	8:A:504:CL:CL	2.56	0.41
1:C:11:GLN:HG3	1:C:74:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:73:ARG:O	4:F:74:LYS:C	2.58	0.41
1:A:251:ASP:OD1	1:A:253:THR:HG22	2.21	0.41
2:B:71:GLU:CG	14:B:612:HOH:O	2.68	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.56	0.41
4:F:221:LEU:HD12	4:F:221:LEU:N	2.34	0.41
4:F:169:LEU:HA	4:F:172:PHE:HB3	2.02	0.41
2:B:288:VAL:N	2:B:289:PRO:HD2	2.35	0.41
2:D:292:THR:HG21	2:D:335:VAL:CG2	2.50	0.41
3:E:92:ASN:O	3:E:96:MET:HG2	2.20	0.41
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.56	0.41
2:B:16:ILE:HD11	2:B:138:THR:HB	2.02	0.41
4:F:146:VAL:CG1	4:F:162:ILE:HG22	2.51	0.41
2:D:395:PHE:CD2	2:D:395:PHE:C	2.95	0.41
4:F:138:ARG:CG	4:F:144:GLY:HA3	2.51	0.41
4:F:348:GLN:O	4:F:351:VAL:CG1	2.69	0.41
1:C:108:TYR:CD2	3:E:108:ASN:CG	2.95	0.40
2:B:88:ARG:NH2	2:B:124:LYS:HD2	2.37	0.40
2:D:147[A]:SER:HB2	2:D:190:SER:HG	1.86	0.40
4:F:305:LYS:HG3	4:F:306:HIS:N	2.37	0.40
1:C:234:ILE:HD13	1:C:302[A]:MET:SD	2.60	0.40
1:C:260:VAL:HA	1:C:261:PRO:HD2	1.95	0.40
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.40	0.40
2:B:172:MET:CE	2:B:203:CYS:SG	3.09	0.40
2:D:71:GLU:HG3	2:D:98:GLY:CA	2.51	0.40
13:F:401:ACP:O2B	13:F:401:ACP:O2G	2.39	0.40
1:A:413:MET:CE	1:A:418:PHE:CE1	3.04	0.40
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/451 (96%)	423 (98%)	9 (2%)	0	100	100
1	C	448/451 (99%)	435 (97%)	13 (3%)	0	100	100
2	B	420/445 (94%)	403 (96%)	17 (4%)	0	100	100
2	D	432/445 (97%)	419 (97%)	13 (3%)	0	100	100
3	E	119/143 (83%)	115 (97%)	2 (2%)	2 (2%)	9	8
4	F	289/384 (75%)	271 (94%)	17 (6%)	1 (0%)	41	50
All	All	2140/2319 (92%)	2066 (96%)	71 (3%)	3 (0%)	51	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	142	GLU
4	F	32	LYS
3	E	27	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	366 (100%)	2 (0%)	88	95
1	C	381/379 (100%)	376 (99%)	5 (1%)	69	82
2	B	367/383 (96%)	363 (99%)	4 (1%)	73	86
2	D	375/383 (98%)	366 (98%)	9 (2%)	49	66
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	273/342 (80%)	267 (98%)	6 (2%)	52	69
All	All	1874/1993 (94%)	1848 (99%)	26 (1%)	69	81

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	334	THR

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Mol	Chain	Res	Type
2	B	139	HIS
2	B	192	HIS
2	B	335	VAL
2	B	345	GLU
1	C	71	GLU
1	C	218	ASP
1	C	302[A]	MET
1	C	302[B]	MET
1	C	381	THR
2	D	2	ARG
2	D	39	ASP
2	D	139	HIS
2	D	179	ASP
2	D	180	THR
2	D	278	ARG
2	D	335	VAL
2	D	345	GLU
2	D	384	ILE
4	F	86	GLU
4	F	186	LEU
4	F	198	LYS
4	F	257	GLU
4	F	265	GLU
4	F	332	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	108	ASN
4	F	260	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 13 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	A	507	-	5,5,5	0.38	0	5,5,5	0.29	0
5	GTP	A	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.79	8 (24%)
10	GDP	D	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.99	8 (25%)
9	GOL	A	506	-	5,5,5	0.32	0	5,5,5	0.35	0
5	GTP	C	501	6	26,34,34	0.90	1 (3%)	33,54,54	1.62	6 (18%)
12	EP	D	504	-	32,36,36	1.32	4 (12%)	39,53,53	1.71	7 (17%)
11	MES	B	504	-	12,12,12	2.32	1 (8%)	14,16,16	1.42	2 (14%)
10	GDP	B	501	6	24,30,30	1.20	2 (8%)	31,47,47	1.94	8 (25%)
11	MES	D	503	-	12,12,12	2.37	1 (8%)	14,16,16	1.55	3 (21%)
13	ACP	F	401	6	27,33,33	1.40	3 (11%)	32,52,52	2.20	7 (21%)
9	GOL	D	505	-	5,5,5	0.35	0	5,5,5	0.16	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	A	507	-	-	2/4/4/4	-
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
10	GDP	D	501	6	-	4/12/32/32	0/3/3/3
9	GOL	A	506	-	-	0/4/4/4	-
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3
12	EP	D	504	-	-	6/49/55/55	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MES	B	504	-	-	1/6/14/14	0/1/1/1
10	GDP	B	501	6	-	5/12/32/32	0/3/3/3
11	MES	D	503	-	-	3/6/14/14	0/1/1/1
13	ACP	F	401	6	-	2/15/38/38	0/3/3/3
9	GOL	D	505	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	MES	C8-S	-8.00	1.66	1.77
11	B	504	MES	C8-S	-7.77	1.66	1.77
10	D	501	GDP	C6-C5	4.03	1.48	1.41
12	D	504	EP	C27-C24	3.99	1.53	1.46
10	B	501	GDP	C6-C5	3.80	1.47	1.41
12	D	504	EP	C72-C68	3.02	1.57	1.53
13	F	401	ACP	C6-N6	2.96	1.44	1.34
13	F	401	ACP	PB-O1B	2.86	1.58	1.51
13	F	401	ACP	C2'-C1'	-2.69	1.49	1.53
5	C	501	GTP	C6-N1	2.59	1.37	1.33
5	A	501	GTP	C6-N1	2.51	1.37	1.33
10	D	501	GDP	C5-C4	2.35	1.47	1.40
12	D	504	EP	C12-N20	2.28	1.44	1.37
10	B	501	GDP	C5-C4	2.09	1.46	1.40
12	D	504	EP	C21-C3	2.08	1.56	1.53

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	401	ACP	O2B-PB-O1B	7.43	134.89	110.07
12	D	504	EP	C27-O26-C24	5.96	64.99	60.69
13	F	401	ACP	O1B-PB-C3B	-5.85	93.60	109.07
5	A	501	GTP	N3-C2-N1	-5.64	119.70	127.22
5	C	501	GTP	N3-C2-N1	-5.11	120.41	127.22
10	B	501	GDP	C2-N3-C4	4.76	120.79	115.36
10	D	501	GDP	C6-C5-C4	-4.73	116.28	120.80
10	D	501	GDP	C6-N1-C2	4.59	123.23	115.93
5	A	501	GTP	C2-N3-C4	4.54	120.55	115.36
10	D	501	GDP	C5-C6-N1	-4.33	117.50	123.43
10	B	501	GDP	C6-C5-C4	-4.24	116.75	120.80
10	B	501	GDP	C6-N1-C2	4.06	122.38	115.93
10	D	501	GDP	C2-N3-C4	4.01	119.93	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	501	GDP	C5-C6-N1	-3.95	118.03	123.43
13	F	401	ACP	N3-C2-N1	-3.89	122.60	128.68
11	B	504	MES	C5-N4-C3	3.80	117.39	108.83
5	C	501	GTP	C2-N3-C4	3.61	119.48	115.36
12	D	504	EP	O26-C24-C27	-3.41	57.47	59.65
11	D	503	MES	O1S-S-C8	3.31	110.90	106.92
12	D	504	EP	O26-C27-C24	-3.31	57.54	59.65
10	B	501	GDP	N3-C2-N1	-3.25	122.89	127.22
10	B	501	GDP	C4-C5-N7	-3.24	106.03	109.40
10	D	501	GDP	N3-C2-N1	-3.18	122.98	127.22
5	C	501	GTP	C5-C6-N1	-3.15	119.13	123.43
10	D	501	GDP	C4-C5-N7	-3.10	106.17	109.40
13	F	401	ACP	PA-O3A-PB	-2.99	123.08	132.56
12	D	504	EP	C16-C15-S1	-2.95	116.14	120.12
10	D	501	GDP	PA-O3A-PB	-2.90	122.88	132.83
11	D	503	MES	C5-N4-C3	2.88	115.31	108.83
5	C	501	GTP	C6-N1-C2	2.77	120.33	115.93
5	A	501	GTP	C6-N1-C2	2.77	120.33	115.93
12	D	504	EP	C53-C51-C47	-2.76	107.76	112.37
5	A	501	GTP	C5-C6-N1	-2.74	119.68	123.43
5	A	501	GTP	PB-O3B-PG	-2.63	123.81	132.83
10	D	501	GDP	C1'-N9-C4	-2.57	122.13	126.64
5	C	501	GTP	PB-O3B-PG	-2.53	124.14	132.83
12	D	504	EP	O2-C75-C72	2.53	116.11	111.46
11	B	504	MES	O2S-S-C8	2.41	109.82	106.92
5	A	501	GTP	PA-O3A-PB	-2.31	124.88	132.83
5	C	501	GTP	PA-O3A-PB	-2.28	125.00	132.83
10	B	501	GDP	O3'-C3'-C4'	-2.27	104.48	111.05
13	F	401	ACP	O2A-PA-O1A	-2.22	101.28	112.24
11	D	503	MES	C6-C5-N4	-2.21	106.75	110.10
13	F	401	ACP	C4-C5-N7	-2.19	107.12	109.40
5	A	501	GTP	C4-C5-N7	-2.15	107.16	109.40
5	A	501	GTP	C6-C5-C4	-2.13	118.76	120.80
12	D	504	EP	C3-O2-C75	2.09	119.49	116.37
10	B	501	GDP	PA-O3A-PB	-2.04	125.84	132.83
13	F	401	ACP	O2B-PB-C3B	-2.01	98.33	106.58

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	501	GDP	C5'-O5'-PA-O1A

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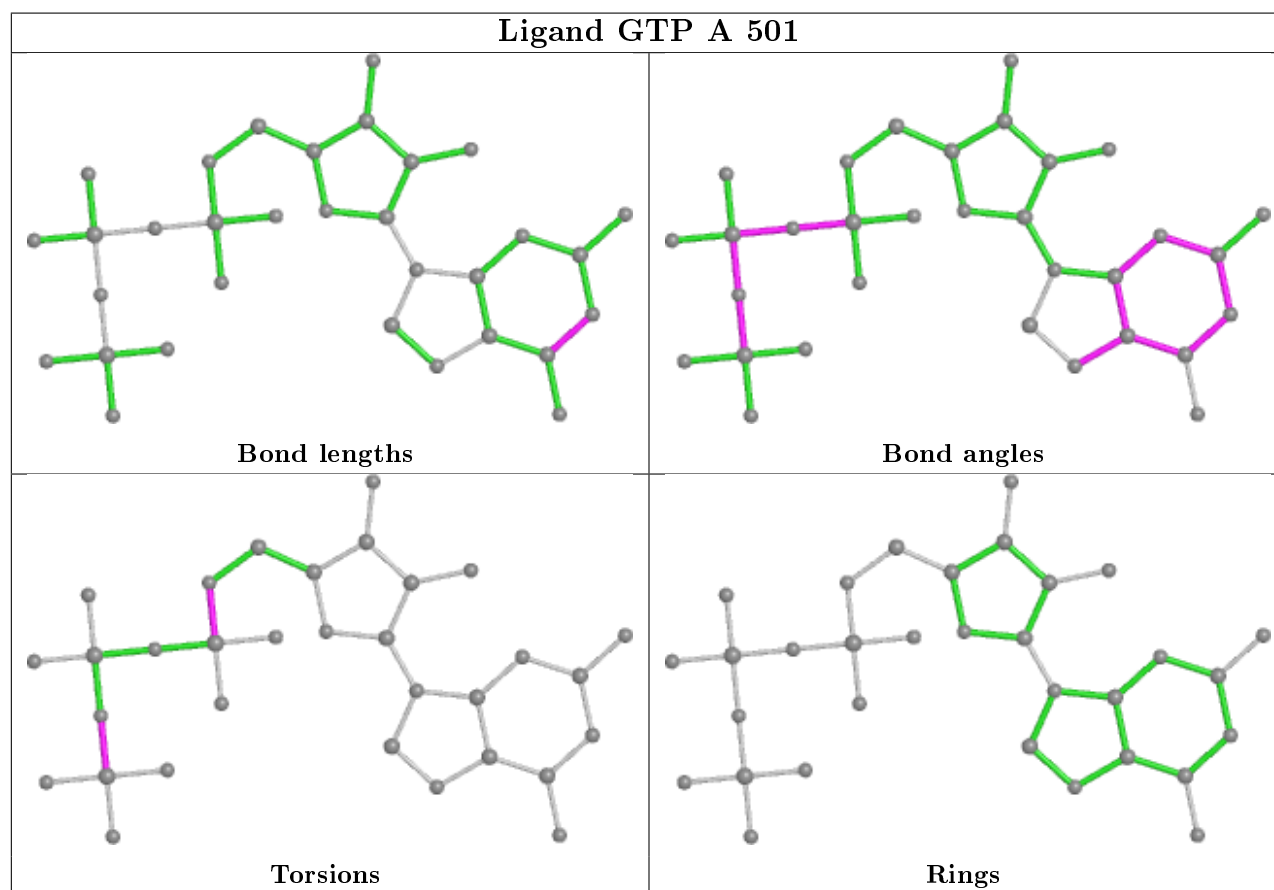
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
12	D	504	EP	C5-C10-C12-N20
12	D	504	EP	C12-C10-C5-C6
12	D	504	EP	C21-C3-C5-C10
11	D	503	MES	C8-C7-N4-C5
11	D	503	MES	N4-C7-C8-S
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
10	B	501	GDP	C5'-O5'-PA-O1A
10	B	501	GDP	C5'-O5'-PA-O2A
9	A	507	GOL	O1-C1-C2-C3
11	B	504	MES	C8-C7-N4-C5
9	D	505	GOL	O1-C1-C2-C3
13	F	401	ACP	O4'-C4'-C5'-O5'
13	F	401	ACP	C3'-C4'-C5'-O5'
9	A	507	GOL	O1-C1-C2-O2
11	D	503	MES	C8-C7-N4-C3
9	D	505	GOL	O1-C1-C2-O2
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
10	D	501	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	PB-O3A-PA-O2A
12	D	504	EP	O2-C3-C5-C10
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
10	B	501	GDP	PB-O3A-PA-O1A
10	B	501	GDP	PB-O3A-PA-O2A
12	D	504	EP	C21-C3-C5-C6
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3B-PG-O3G
10	D	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
10	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
12	D	504	EP	C12-C10-C5-C3

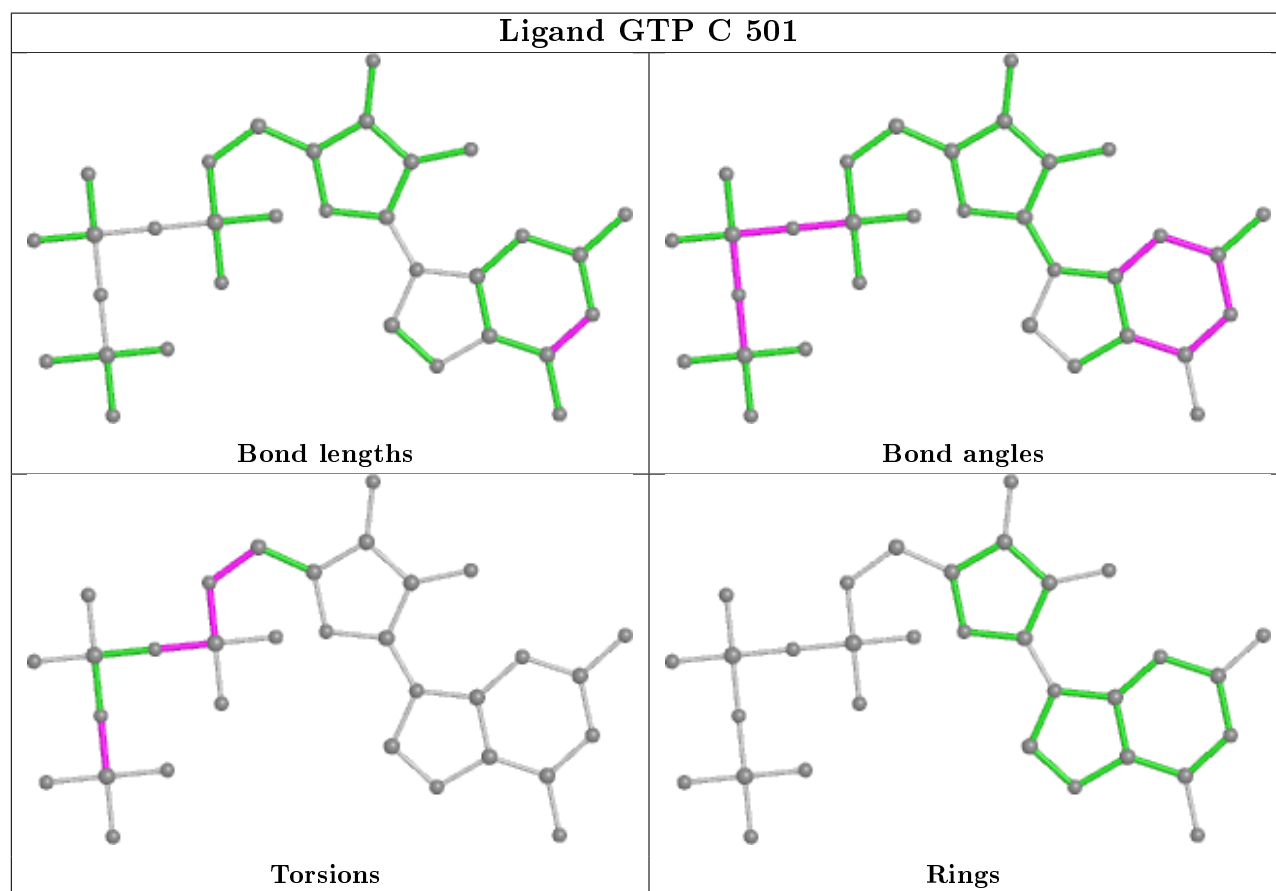
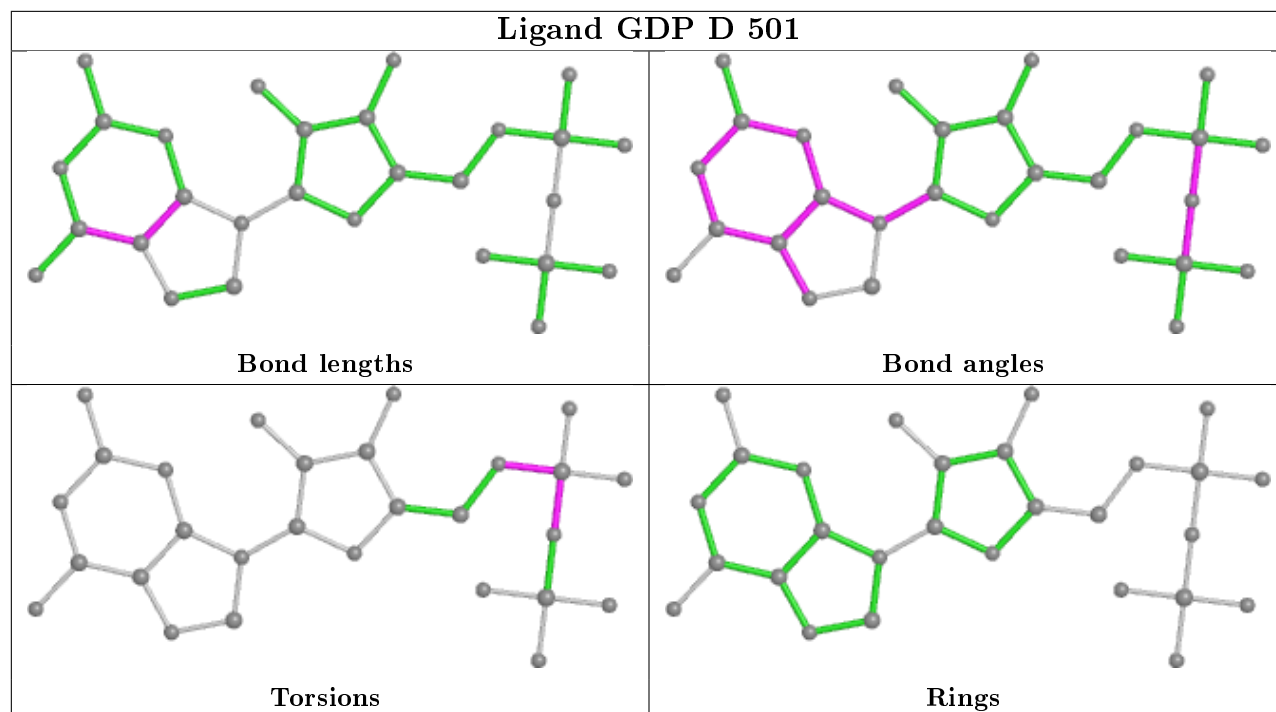
There are no ring outliers.

6 monomers are involved in 9 short contacts:

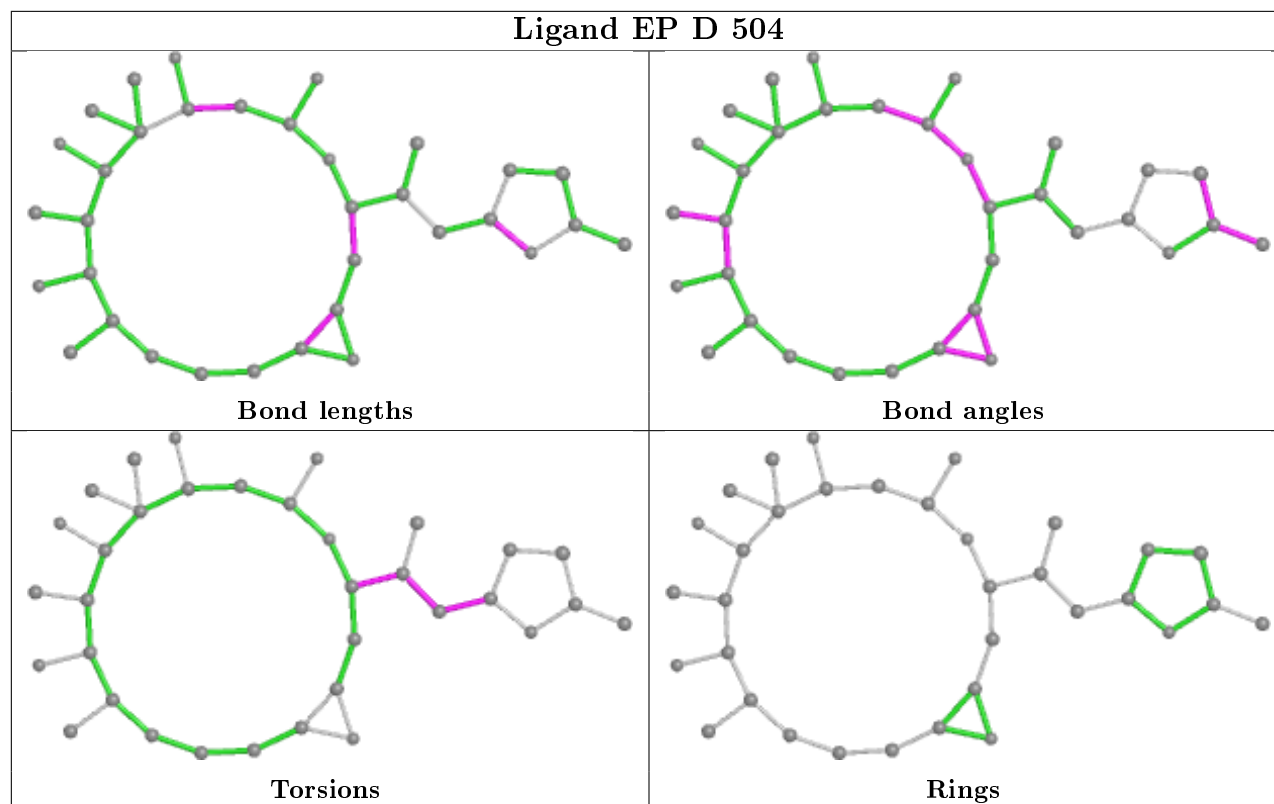
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	501	GDP	1	0
12	D	504	EP	1	0
11	B	504	MES	2	0
10	B	501	GDP	1	0
11	D	503	MES	2	0
13	F	401	ACP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

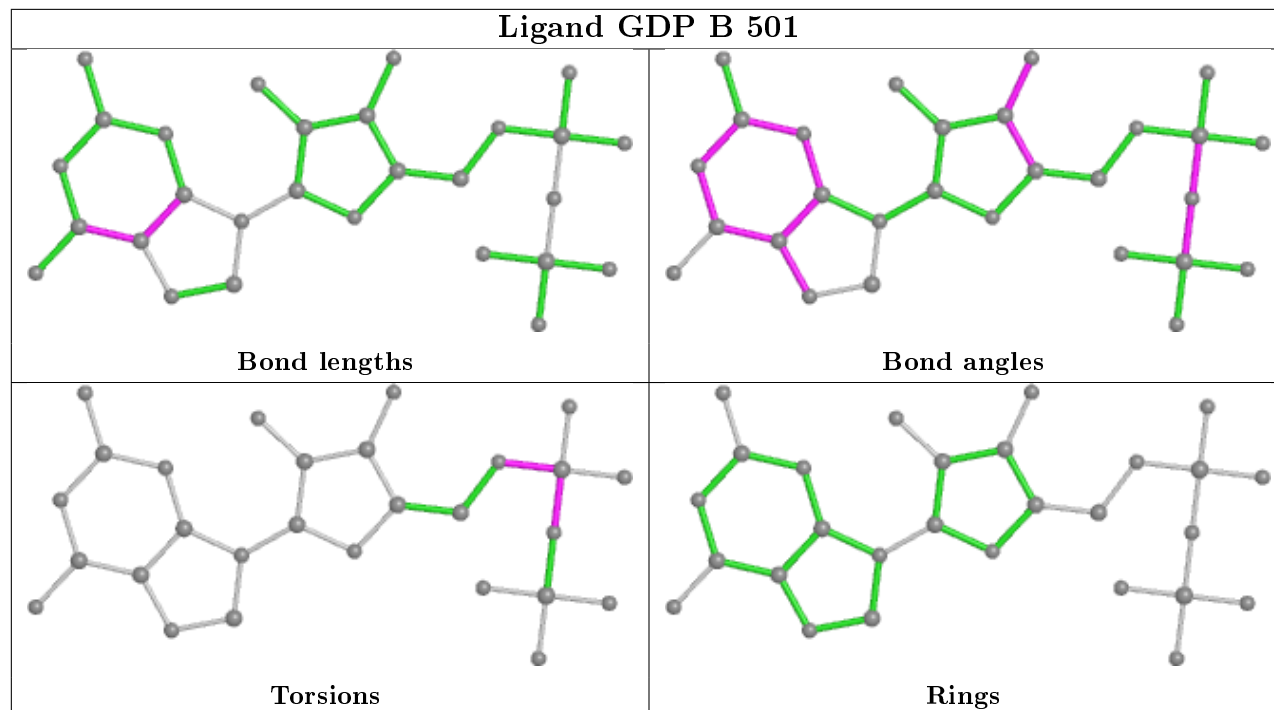


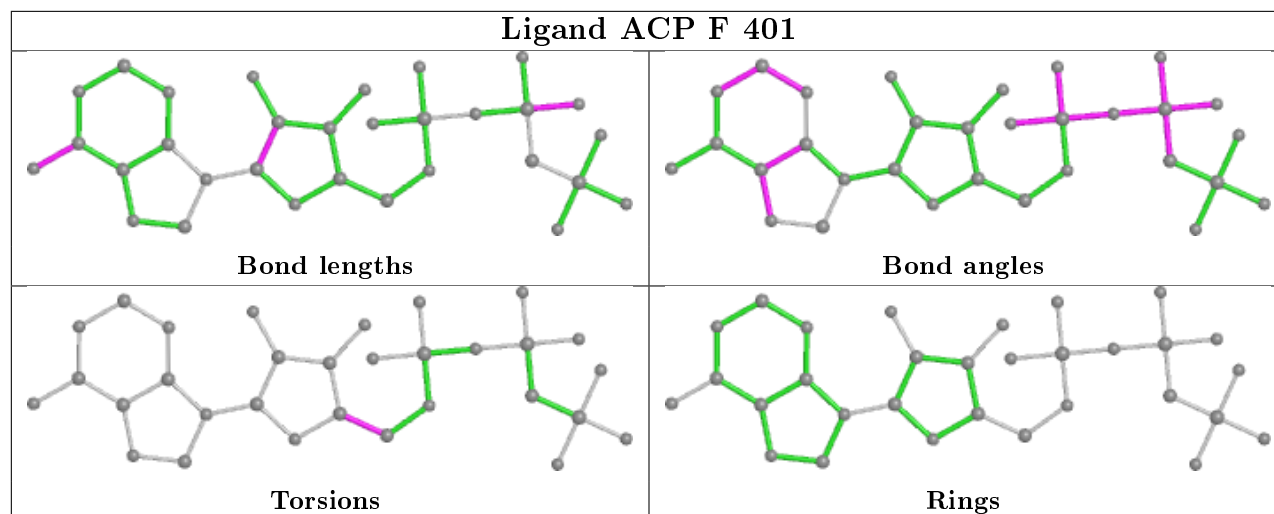


Ligand EP D 504



Ligand GDP B 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	436/451 (96%)	0.27	0 100 100	32, 56, 95, 127	0
1	C	440/451 (97%)	0.46	6 (1%) 75 80	32, 47, 81, 148	0
2	B	422/445 (94%)	0.54	16 (3%) 40 47	36, 57, 100, 160	5 (1%)
2	D	430/445 (96%)	0.34	7 (1%) 72 77	34, 61, 100, 169	4 (0%)
3	E	123/143 (86%)	0.48	4 (3%) 46 53	38, 71, 115, 129	0
4	F	303/384 (78%)	1.17	67 (22%) 0 1	44, 80, 155, 221	0
All	All	2154/2319 (92%)	0.52	100 (4%) 32 39	32, 59, 110, 221	9 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	8.8
4	F	134	ALA	8.8
4	F	138	ARG	8.4
4	F	173	ILE	6.8
4	F	137	ARG	5.8
4	F	186	LEU	5.7
4	F	147	TRP	5.4
4	F	169	LEU	4.8
4	F	162	ILE	4.7
4	F	182	ILE	4.7
4	F	192	LEU	4.7
4	F	245	ILE	4.6
2	D	401	ARG	4.4
2	B	337	ASN	4.2
2	B	276	THR	4.1
2	B	57	THR	4.0
4	F	199	PHE	4.0
4	F	242	ASN	4.0
4	F	143	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	333	LEU	3.8
4	F	224	SER	3.8
2	B	439	THR	3.8
4	F	21	LEU	3.8
4	F	223	THR	3.7
2	B	440	ALA	3.7
4	F	179	VAL	3.6
2	D	400	ARG	3.5
4	F	181	VAL	3.5
4	F	372	THR	3.4
2	B	322	ARG	3.4
4	F	335	ALA	3.3
4	F	258	GLU	3.3
4	F	150	LYS	3.3
4	F	148	ILE	3.3
2	B	338	LYS	3.3
4	F	146	VAL	3.2
4	F	133	ALA	3.1
4	F	283	ILE	3.1
4	F	247	LYS	3.1
1	C	1	MET	3.1
4	F	362	ALA	3.1
4	F	330	ILE	3.1
2	D	405	LEU	3.0
2	B	358	ILE	2.9
4	F	22	LEU	2.9
4	F	172	PHE	2.9
1	C	357	TYR	2.8
3	E	26	PRO	2.8
4	F	20	LEU	2.7
4	F	180	HIS	2.7
4	F	243	HIS	2.7
4	F	201	ILE	2.7
4	F	198	LYS	2.7
4	F	73	ARG	2.7
1	C	340	SER	2.6
4	F	257	GLU	2.6
4	F	36	ARG	2.5
4	F	343	TYR	2.5
4	F	261	GLU	2.5
4	F	46	ARG	2.5
4	F	361	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	132	LEU	2.4
4	F	28	LYS	2.4
4	F	260	ASN	2.4
4	F	319	PHE	2.4
4	F	31	ARG	2.4
4	F	221	LEU	2.4
2	B	49	ILE	2.3
4	F	256	TYR	2.3
2	D	179	ASP	2.3
4	F	149	ALA	2.3
4	F	317	PHE	2.3
1	C	335	ILE	2.3
2	B	248	LEU	2.3
1	C	179	THR	2.3
4	F	135	TYR	2.3
4	F	267	PHE	2.2
1	C	302[A]	MET	2.2
4	F	336	PRO	2.2
3	E	24	LEU	2.2
3	E	128	LYS	2.2
4	F	264	PHE	2.2
4	F	248	GLU	2.2
2	B	42	LEU	2.2
2	D	153	LEU	2.2
2	B	335	VAL	2.1
4	F	139	ARG	2.1
4	F	175	GLU	2.1
4	F	320	MET	2.1
2	B	336	GLN	2.1
2	D	248	LEU	2.1
4	F	285	LEU	2.1
2	D	94	PHE	2.1
3	E	45	PRO	2.1
4	F	376	ILE	2.1
4	F	44	ARG	2.0
2	B	372	LYS	2.0
2	B	288	VAL	2.0
4	F	163	SER	2.0
4	F	341	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

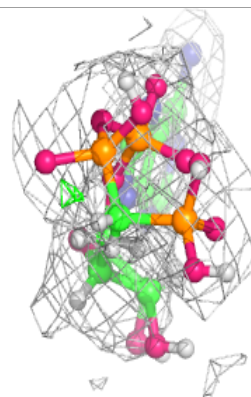
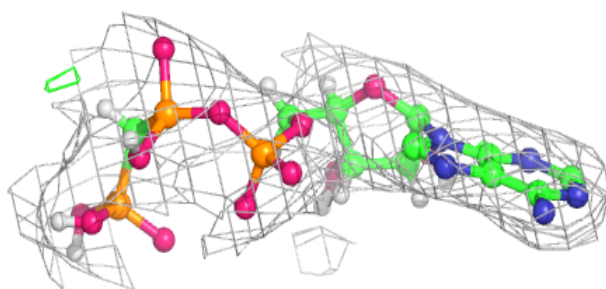
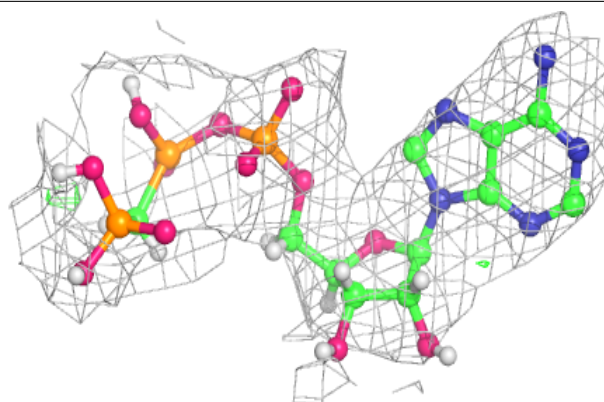
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	502	1/1	0.76	0.20	58,58,58,58	0
7	CA	C	504	1/1	0.81	0.35	116,116,116,116	0
7	CA	C	505	1/1	0.83	0.35	97,97,97,97	0
8	CL	A	504	1/1	0.83	0.14	73,73,73,73	0
9	GOL	D	505	6/6	0.83	0.28	83,109,119,132	0
6	MG	F	403	1/1	0.86	0.17	97,97,97,97	0
6	MG	F	402	1/1	0.86	0.51	126,126,126,126	0
13	ACP	F	401	31/31	0.86	0.20	63,97,118,143	0
7	CA	B	503	1/1	0.87	0.33	91,91,91,91	0
9	GOL	A	506	6/6	0.89	0.14	54,74,97,106	0
6	MG	D	502	1/1	0.89	0.19	56,56,56,56	0
9	GOL	A	507	6/6	0.90	0.15	57,90,114,114	0
11	MES	D	503	12/12	0.91	0.41	87,108,149,155	0
7	CA	A	505	1/1	0.91	0.23	97,97,97,97	0
7	CA	C	503	1/1	0.92	0.28	72,72,72,72	0
12	EP	D	504	34/34	0.95	0.17	38,67,90,100	0
6	MG	C	502	1/1	0.95	0.23	39,39,39,39	0
11	MES	B	504	12/12	0.97	0.14	52,67,89,94	0
10	GDP	D	501	28/28	0.98	0.14	41,53,69,74	0
5	GTP	C	501	32/32	0.98	0.17	25,35,46,51	0
7	CA	A	503	1/1	0.98	0.21	72,72,72,72	0
5	GTP	A	501	32/32	0.98	0.18	28,42,56,60	0
10	GDP	B	501	28/28	0.99	0.20	22,39,50,72	0
6	MG	B	502	1/1	0.99	0.24	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

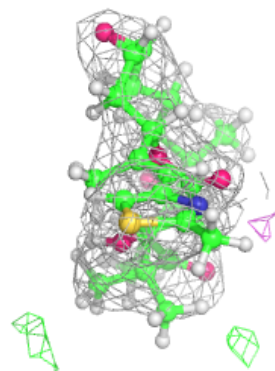
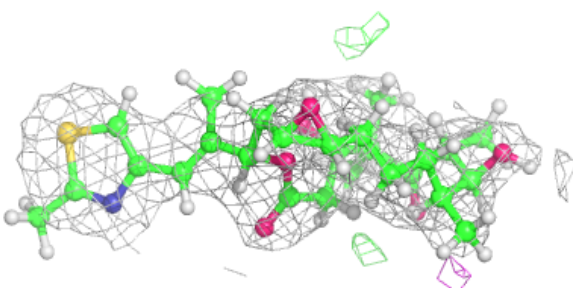
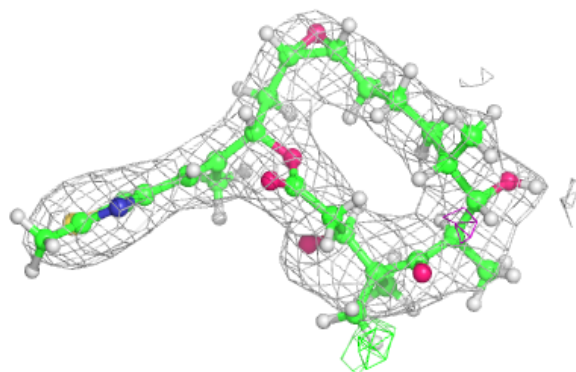
Electron density around ACP F 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



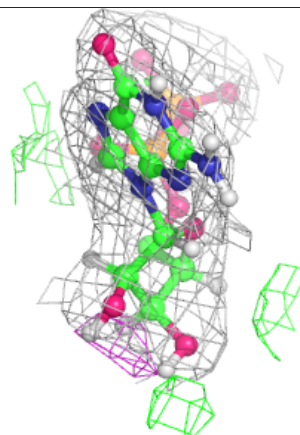
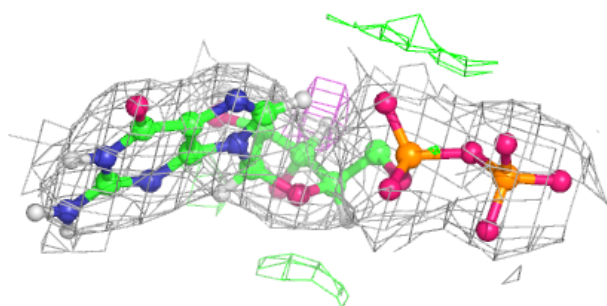
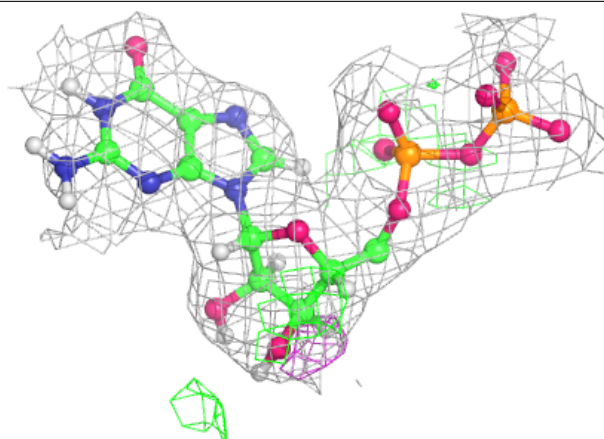
Electron density around EP D 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

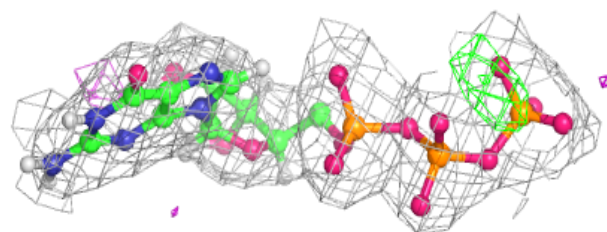
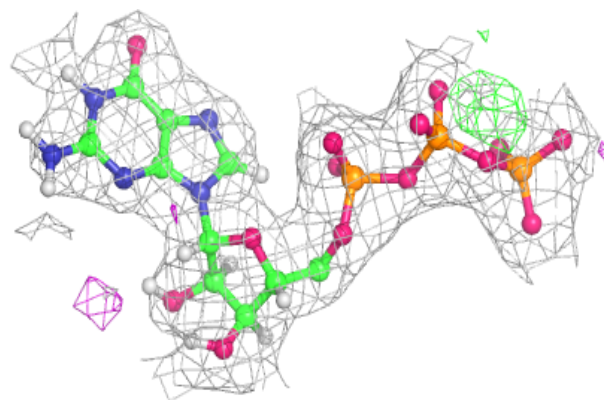


Electron density around GDP D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

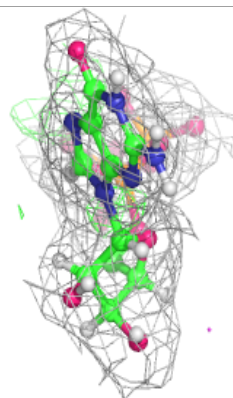
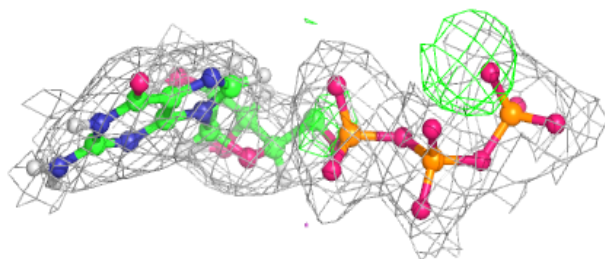
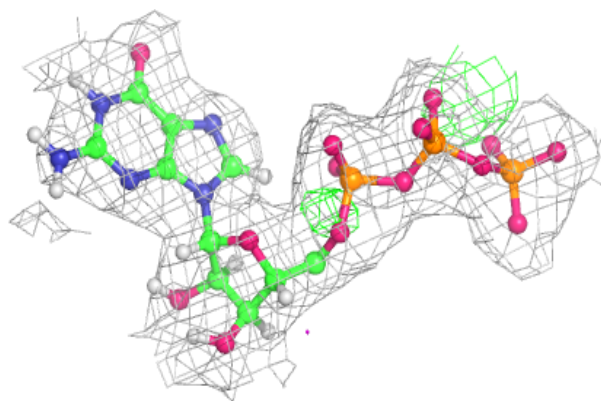
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



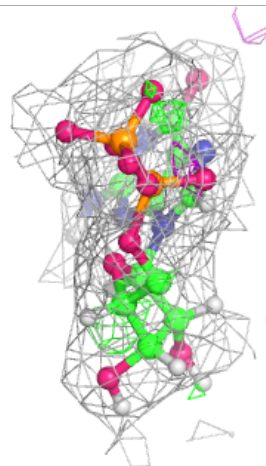
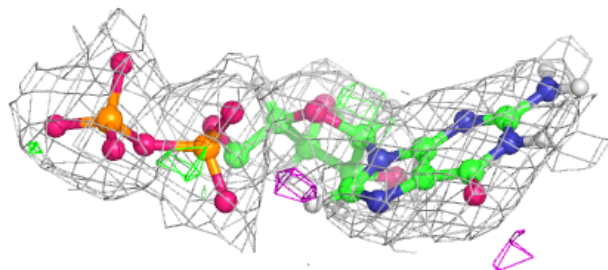
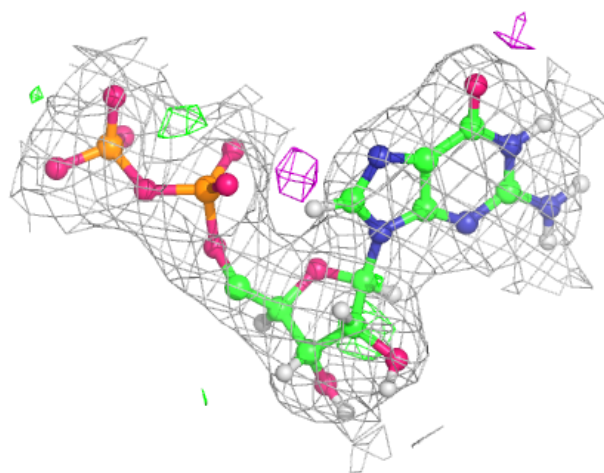
Electron density around GTP A 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDP B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.